For the concentrated solutions, τ_3 (3.50 psec at 20°C for 0.1738 mole-fraction) is of the same order as that obtained for OH-group in pure *n*-octanol by Garg & Smyth (1965) and is temperature dependent. τ_1 (652 psec at 20°C for 0 1738 mole-fraction) is large and may be due to the rupture of hydrogen bonds inside the associated chain τ_2 (34 psec for the same concentration and temperature) has about the same value as τ_1 in the dilute solutions should be connected with the rotation of the single molecules or to the ones at the end of the associated chains. G_3 increases with the increase in temperature which demonstrates the decomposition or loosening of the association with increase in temperature

From figure 1 and the results of analysis, it is clear that associates are formed because the OH-group lies at the end of the chain and hence is subjected to intermolecular interaction, unlike the case of 3,5-dimethyl 3-hexanol (Hanna & Abdel-Nour 1970) where the associates are hardly detectable as the OH-group lies within the molecule and is shielded against the intermolecular interaction

Detailed results will be given after measuring ϵ' and ϵ'' at meter waves to subtract the contribution of the lower dispersion region from the microwave measurements for accurate evaluation of the results

The authors thank Prof M. Mokhtar for his encouragement and to Prof C. P Smyth for allowing one of us (Abdel-Nour) to take the measurements in his laboratory.

References

Garg, S. K. & Smyth, C. P 1965 *J Phys. Chem.* 69, 1294
Hanna, F. F. & Abdel-Nour, K. N. 1970 under preparation for publication.

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X-ray crystallographic data for some organic compounds

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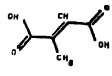
As a part of programme for determining structures of simple organic molecules and their derivatives, we have investigated a number of molecules and the present note reports some preliminary results

1. *Potassium mesaconate* $KC_5H_5O_4$.

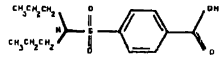
This is acid potassium salt of the dicarboxylic mesaconic acid $C_5H_6O_4$ with stereochemical formula;



The crystal is transparent and platy in habit, belonging to the triclinic system with $a = 6.23$Å, $b = 7.33$Å, $c = 3.97$Å, $\alpha = 87° 36'$, $\beta = 107° 30'$, $\gamma = 98° 20'$, $V = 170.95$Å^3 $\rho_{calc} = 1.63$ gm/ml, $\rho_{obs} = 1.62$ gm/ml. Number of molecules in the unit cell $Z = 1$. Linear absorption coefficient for copper K_α radiation $= 63.99$ cm^{-1}. As there is only one molecule in the unit cell and the molecule itself is noncentrosymmetric, the space group is uniquely fixed as $P1$. Complete zonal and three dimensional X-ray data have been collected using Weissenberg photography and the structure solved in projections. Refinement of the structure by three-dimensional least squares is in progress

2 *Probenecid* $C_{13}H_{19}O_4NS$

This is a monocarboxylic acid with the stereochemical formula:



and crystallizes out of a solution in chloroform. The crystal is platy and colourless and belongs to the triclinic system with $a = 7.53$Å, $b = 19.51$Å, $c = 5.31$Å, $\alpha = 102° 8'$, $\beta = 99° 6'$, $\gamma = 93° 5'$, $V = 750.4$ Å^3 and $\rho_{calc} = 1.27$ gm/ml. $\rho_{obs} = 1.25$ gm/ml. The number of molecules in the unit cell $Z = 2$. Linear absorption coefficient for CuK_α radiation $\mu = 19.56$ cm^{-1}. Statistical intensity tests, morphology and number of furmula units in the cell all indicate the space group to be centrosymmetric $P\bar{1}$. We have collected complete zonal and three-dimensional X-ray diffraction data using Weissenberg photography, and a three-dimensional Patterson synthesis is now in progress to locate the sulphur atom.

3. *O-Aceto benzoic acid* $C_9H_8O_3$

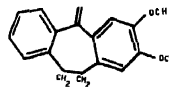
It is crystallized out of a solution in alcohol in the form of elongated plate. The stereochemical formula of the compound is

The crystal is orthorhombic with $a = 9.53$Å, $b = 5.22$Å. $c = 15.82$Å, $V = 787.0$Å^3 $\rho_{calc} = 1.38$ gm/ml, $\rho_{obs} = 1.36$ gm/ml The number of molecules in the unit cell $Z = 4$. Linear absorption coefficient for copper K_α radiation $\mu = 8.88$ cm^{-1}. The only space group absences are $h00$, $h = 2n+1$, $0k0$, $k = 2n+1$, $00l$, $l = 2n+1$,

This fixes the space group uniquely as $P2_12_12_1$. The crystal structure investigation is in progress

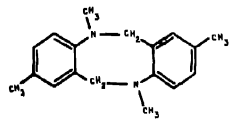
4 *Dimethoxy di-benzo suberone* $C_{17}H_{16}O_3$.

The compound with the stereochemical formula



is of interest because of the central seven-membered ring. The crystal is needle shaped and orthorhombic with $a = 16.56$ Å, $b = 21.48$Å and $c = 7.56$Å, $\rho_{calc} = 1.322$ gm/ml, $\rho_{obs} = 1.285$ gm/ml. The number of molecules in the unit cell $Z = 8$ The linear absorption co-efficient for copper K_α radiation $\mu = 7.38$ cm^{-1}. The space group absences are $0kl$ with $k = 2n+1$, $h0l$ with $l = 2n+1$ and $hk0$ with $h = 2n+1$. This fixes the space group uniquely as *Pbca*. We have collected complete three-dimensional X-ray diffraction data with Weissenberg photography and obtained an approximate solution for the structure. Since we suspect disorder in the structure it is still under our investigation

5. 1-*methyl* 9-*methyl* 5, 6, 11, 12-*tri-hydro* 5, 11-*dimethylphenhomazine* $C_{16}H_{20}N_2$. The compound with the stereochemical formula



is of interest because of the central eight-membered ring The crystal is platy in habit and belongs to the monoclinic system, with $a = 10.13$Å, $b = 7.36$Å, $c = 20.66$Å, $\beta = 105° 40'$, $V = 1483.1$Å^3 $\rho_{calc} = 1.18$ gm/ml. Number of molecules in the unit cell $Z = 4$ The linear absorption coefficient for copper K_α radiation $\mu = 8.43$ cm^{-1}. Space group absences are $h0l$ when $l = 2n+1$, $0k0$ when $k = 2n+1$. This fixes the space group uniquely as $P2_1/c$. We have collected complete three-dimensional *X*-ray diffraction data for the compound using Weissenberg photography and got an approximate solution of its structure in the $0kl$ projection. Further work to refine the structure is in progress.